Quantum algorithms for Nuclear Physics I

Dean Lee
Facility for Rare Isotope Beams
Michigan State University

Co-ordinated Mini-Lecture Series on
Quantum Computing and Quantum Information Science
for Nuclear Physics

Jefferson Laboratory
March 16, 2020

Outline

Qubits

Bloch sphere

Single-qubit gates

Two-qubit gates

Jordan-Wigner transformation

Quantum Fourier transform

Quantum circuits and performance

Lattice methods for nuclear physics

Qubits

The basic element in quantum computation is the qubit, which is a simply a two-level quantum system.

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

There are also extensions to systems with more than two levels, known as qudits. But we will focus on qubits in these lectures.

In general, our qubit will be in a general superposition of the two states.

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle \qquad |\psi\rangle = \alpha \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \beta \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

With proper normalization we have

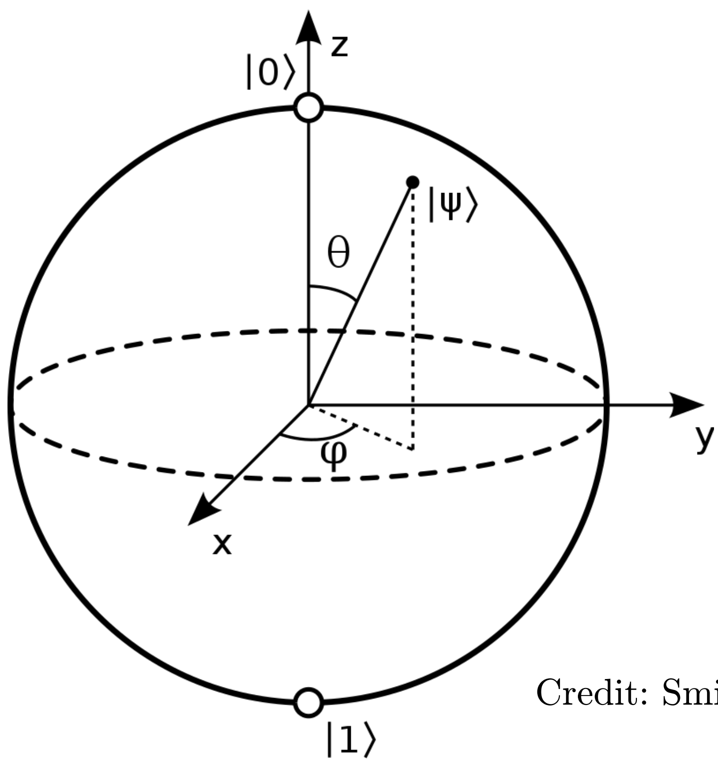
$$|\alpha|^2 + |\beta|^2 = 1$$

Up to an overall complex phase, we can write

$$|\psi\rangle = \cos(\theta/2)\,|0\rangle + e^{i\varphi}\sin(\theta/2)\,|1\rangle$$

$$0 \leq \theta \leq \pi,\ 0 \leq \varphi < 2\pi$$

This can be represented as a point on the Bloch sphere



Credit: Smite-Meister

For a two-qubit system we have the four basis states

$$|00\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \qquad |01\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \qquad |10\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \qquad |11\rangle = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

Any arbitrary state can be written as

$$|\psi\rangle = \alpha_{00}\,|00\rangle + \alpha_{01}\,|01\rangle + \alpha_{10}\,|10\rangle + \alpha_{11}\,|11\rangle$$

with normalization

$$|\alpha_{00}|^2 + |\alpha_{01}|^2 + |\alpha_{10}|^2 + |\alpha_{11}|^2 = 1$$

For the N-qubit system, any arbitrary state can be written as

$$|\psi\rangle = \sum_{i_1 \in \{0,1\}} \cdots \sum_{i_N \in \{0,1\}} \alpha_{i_1 \cdots i_N} |i_1 \cdots i_N\rangle$$

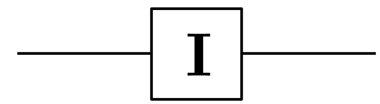
with normalization

$$\sum_{i_1 \in \{0,1\}} \cdots \sum_{i_N \in \{0,1\}} |\alpha_{i_1 \cdots i_N}|^2 = 1$$

Single-Qubit Gates

Since the evolution of quantum systems is unitary, all quantum gates are unitary.

Identity gate



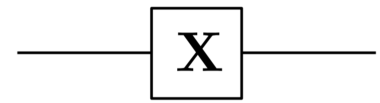
$$\mathbf{I}\left|0\right\rangle = \left|0\right\rangle,\ \mathbf{I}\left|1\right\rangle = \left|1\right\rangle$$

$$\mathbf{I} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

$$\mathbf{I}^{\dagger} = \mathbf{I} = \mathbf{I}^{-1}$$

NOT gate (= Pauli-X gate)



If we view 0 and 1 as logical false and true, then the NOT gate corresponds to a logical negation or bit flip that exchanges 0 and 1.

$$\mathbf{X}\left|0\right\rangle = \left|1\right\rangle, \ \mathbf{X}\left|1\right\rangle = \left|0\right\rangle$$

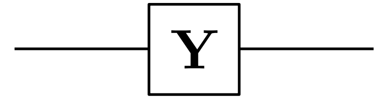
$$\mathbf{X} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} \beta \\ \alpha \end{bmatrix}$$

$$\mathbf{X}^{\dagger} = \mathbf{X} = \mathbf{X}^{-1}$$

The **X** notation for NOT has a double meaning, since **X** can also be viewed as the Pauli-X gate.

Pauli-Y gate

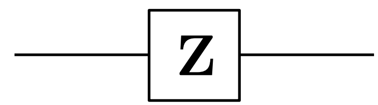


$$\mathbf{Y} = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

$$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} -i\beta \\ i\alpha \end{bmatrix}$$

$$\mathbf{Y}^\dagger = \mathbf{Y} = \mathbf{Y}^{-1}$$

Pauli-Z gate

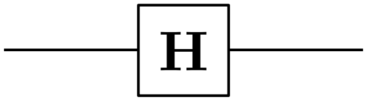


$$\mathbf{Z} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} \alpha \\ -\beta \end{bmatrix}$$

$$\mathbf{Z}^\dagger = \mathbf{Z} = \mathbf{Z}^{-1}$$

Hadamard gate

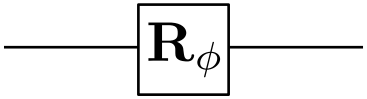


$$\mathbf{H}\left|0\right\rangle = \frac{1}{\sqrt{2}}\left|0\right\rangle + \frac{1}{\sqrt{2}}\left|1\right\rangle,\ \mathbf{H}\left|1\right\rangle = \frac{1}{\sqrt{2}}\left|0\right\rangle - \frac{1}{\sqrt{2}}\left|1\right\rangle$$

$$\mathbf{H} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}$$

$$\mathbf{H}^{\dagger} = \mathbf{H} = \mathbf{H}^{-1}$$

Phase gate



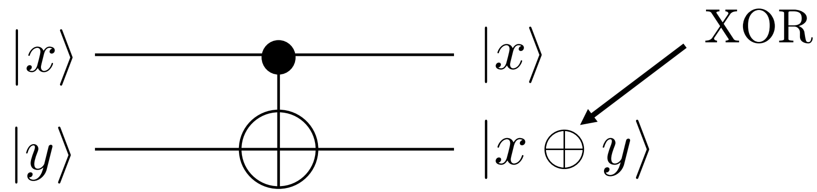
$$\mathbf{R}_\phi\left|0\right\rangle = \left|0\right\rangle,\ \mathbf{R}_\phi\left|1\right\rangle = e^{i\phi}\left|1\right\rangle$$

$$\mathbf{R}_\phi = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{bmatrix}$$

$$\mathbf{R}_\phi^{\dagger} = \mathbf{R}_{-\phi} = \mathbf{R}_\phi^{\mathbf{-1}}$$

Two-Qubit Gates

Controlled-NOT (C-NOT) gate

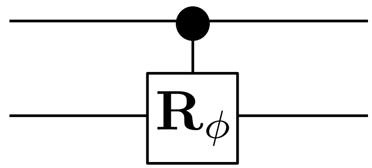


$$|00\rangle \to |00\rangle \qquad |01\rangle \to |01\rangle \qquad |10\rangle \to |11\rangle \qquad |11\rangle \to |10\rangle$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

$$|00\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \qquad |01\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \qquad |10\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \qquad |11\rangle = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

Controlled Phase gate

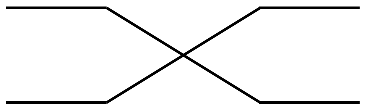


$$|00\rangle \to |00\rangle \qquad |01\rangle \to |01\rangle \qquad |10\rangle \to |10\rangle \qquad |11\rangle \to e^{i\phi}|11\rangle$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\phi} \end{bmatrix}$$

$$|00\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \qquad |01\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \qquad |10\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \qquad |11\rangle = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

SWAP gate



$$|00\rangle \rightarrow |00\rangle \qquad |01\rangle \rightarrow |10\rangle \qquad |10\rangle \rightarrow |01\rangle \qquad |11\rangle \rightarrow |11\rangle$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$|00\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \qquad |01\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \qquad |10\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \qquad |11\rangle = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

Jordan-Wigner transformation

Our qubit basis states

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

are reminiscent of the possible occupation numbers of a fermionic particle.

To make this connection exact, we also need to incorporate Fermi/Dirac statistics. The Jordan-Wigner transformation is one way to encode this information.

Suppose we have a system of qubits then we can write

$$a_k = \mathbf{Z}_1 \cdots \mathbf{Z}_{k-1}(\mathbf{X}_k/2 + i\mathbf{Y}_k/2)$$
$$a_k^\dagger = \mathbf{Z}_1 \cdots \mathbf{Z}_{k-1}(\mathbf{X}_k/2 - i\mathbf{Y}_k/2)$$

Therefore fermionic bilinear have the form

$$a_k^\dagger a_{k+n} = \mathbf{Z}_k \cdots \mathbf{Z}_{k+n-1}(\mathbf{X}_k/2 - i\mathbf{Y}_k/2)(\mathbf{X}_{k+n}/2 + i\mathbf{Y}_{k+n}/2)$$

$$a_{k+n}^\dagger a_k = \mathbf{Z}_k \cdots \mathbf{Z}_{k+n-1}(\mathbf{X}_{k+n}/2 - i\mathbf{Y}_{k+n}/2)(\mathbf{X}_k/2 + i\mathbf{Y}_k/2)$$

Quantum Fourier transform

In the following we are discussing discrete Fourier transforms. We let N be a power of 2

$$N = 2^n$$

The classical Fourier transform acts on a string of N complex numbers

$$(a_0, a_1, \cdots, a_{N-1}) \in C^N$$

and outputs another string of N complex numbers

$$(b_0, b_1, \cdots, b_{N-1}) \in C^N$$

according to the rule

$$b_k = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} a_j \omega_N^{kj} \qquad \omega_N = e^{2\pi i/N}$$

The quantum Fourier transform acts on a quantum state as

$$\text{QFT} : \sum_{j=0}^{N-1} a_j \left| j \right\rangle \rightarrow \sum_{j=0}^{N-1} b_j \left| j \right\rangle$$

where

$$b_k = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} a_j \omega_N^{kj}$$

In matrix form the unitary matrix we need is

$$F_N = \frac{1}{\sqrt{N}} \begin{bmatrix} 1 & 1 & 1 & 1 & \cdots & 1 \\ 1 & \omega & \omega^2 & \omega^3 & \cdots & \omega^{N-1} \\ 1 & \omega^2 & \omega^4 & \omega^6 & \cdots & \omega^{2(N-1)} \\ 1 & \omega^3 & \omega^6 & \omega^9 & \cdots & \omega^{2(N-1)} \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ 1 & \omega^{N-1} & \omega^{(N-1)2} & \omega^{(N-1)3} & \cdots & \omega^{(N-1)(N-1)} \end{bmatrix}$$

When building a quantum circuit that produces this unitary transformation, it suffices to show that the transformation is correct for each of the N basis states

$$|j\rangle = |0\rangle , \cdots , |2^n - 1\rangle$$

We represent the integer j in binary representation

$$j = j_1 2^{n-1} + j_2 2^{n-2} \cdots + j_n 2^0 = [j_1 j_2 \cdots j_n]$$

Using this binary representation we can write our basis as tensor product of qubits

$$|j\rangle = |j_1 j_2 \cdots j_n\rangle = |j_1\rangle \otimes |j_2\rangle \otimes \cdots \otimes |j_n\rangle$$

It is also convenient to use the fractional binary notation

$$[0.j_1 \cdots j_m] = \sum_{k=1}^{m} j_k 2^{-k}$$

So that, for example,

$$[0.j_1] = \frac{j_1}{2} \qquad [0.j_1 j_2] = \frac{j_1}{2} + \frac{j_2}{2^2}$$

We will show that

$$\mathrm{QFT}(|j_1 j_2 \cdots j_n\rangle) =$$

$$\frac{1}{\sqrt{N}}(|0\rangle + e^{2\pi i[0.j_n]}|1\rangle) \otimes (|0\rangle + e^{2\pi i[0.j_{n-1}j_n]}|1\rangle) \otimes \cdots \otimes (|0\rangle + e^{2\pi i[0.j_1 j_2 \cdots j_n]}|1\rangle)$$

$$
\begin{aligned}
\mathrm{QFT}(|j_1 j_2 \cdots j_n\rangle) &= \frac{1}{\sqrt{N}} \sum_{k=0}^{2^n-1} \omega_N^{jk} |k\rangle \\
&= \frac{1}{\sqrt{N}} \sum_{k_1=0,1} \cdots \sum_{k_n=0,1} \omega_N^{j \sum_{l=1}^{n} k_l 2^{n-l}} |k_1 k_2 \cdots k_n\rangle \\
&= \frac{1}{\sqrt{N}} \sum_{k_1=0,1} \cdots \sum_{k_n=0,1} \bigotimes_{l=1}^{n} \omega_N^{jk_l 2^{n-l}} |k_l\rangle \\
&= \frac{1}{\sqrt{N}} \sum_{k_1=0,1} \cdots \sum_{k_n=0,1} \omega_N^{jk_1 2^{n-1}} |k_1\rangle \otimes \bigotimes_{l=2}^{n} \omega_N^{jk_l 2^{n-l}} |k_l\rangle \\
&= \frac{1}{\sqrt{N}} \left(\sum_{k_1=0,1} \omega_N^{jk_1 2^{n-1}} |k_1\rangle \right) \otimes \sum_{k_2=0,1} \cdots \sum_{k_n=0,1} \bigotimes_{l=2}^{n} \omega_N^{jk_l 2^{n-l}} |k_l\rangle \\
&= \frac{1}{\sqrt{N}} \bigotimes_{l=1}^{n} \sum_{k_l=0,1} \omega_N^{jk_l 2^{n-l}} |k_l\rangle \\
&= \frac{1}{\sqrt{N}} \bigotimes_{l=1}^{n} \left(|0\rangle + \omega_N^{j 2^{n-l}} |1\rangle \right)
\end{aligned}
$$

So far we have shown

$$\mathrm{QFT}(|j_1 j_2 \cdots j_n\rangle) = \frac{1}{\sqrt{N}} \bigotimes_{l=1}^{n} \left(|0\rangle + \omega_N^{j2^{n-l}} |1\rangle \right)$$

We note that

$$\omega_N^{j2^{n-l}} = e^{\frac{2\pi i}{2^n} j2^{n-l}} = e^{2\pi i j 2^{-l}}$$

Only the fractional part of $j2^{-l}$ needs to be kept since the integer part produces a factor of 1. For example,

$$\omega_N^{j2^{n-1}} = e^{2\pi i [0.j_n]} \qquad \omega_N^{j2^{n-2}} = e^{2\pi i [0.j_{n-1} j_n]}$$

In the general case

$$\omega_N^{j2^{n-l}} = e^{2\pi i [0.j_{n-l+1} \cdots j_n]}$$

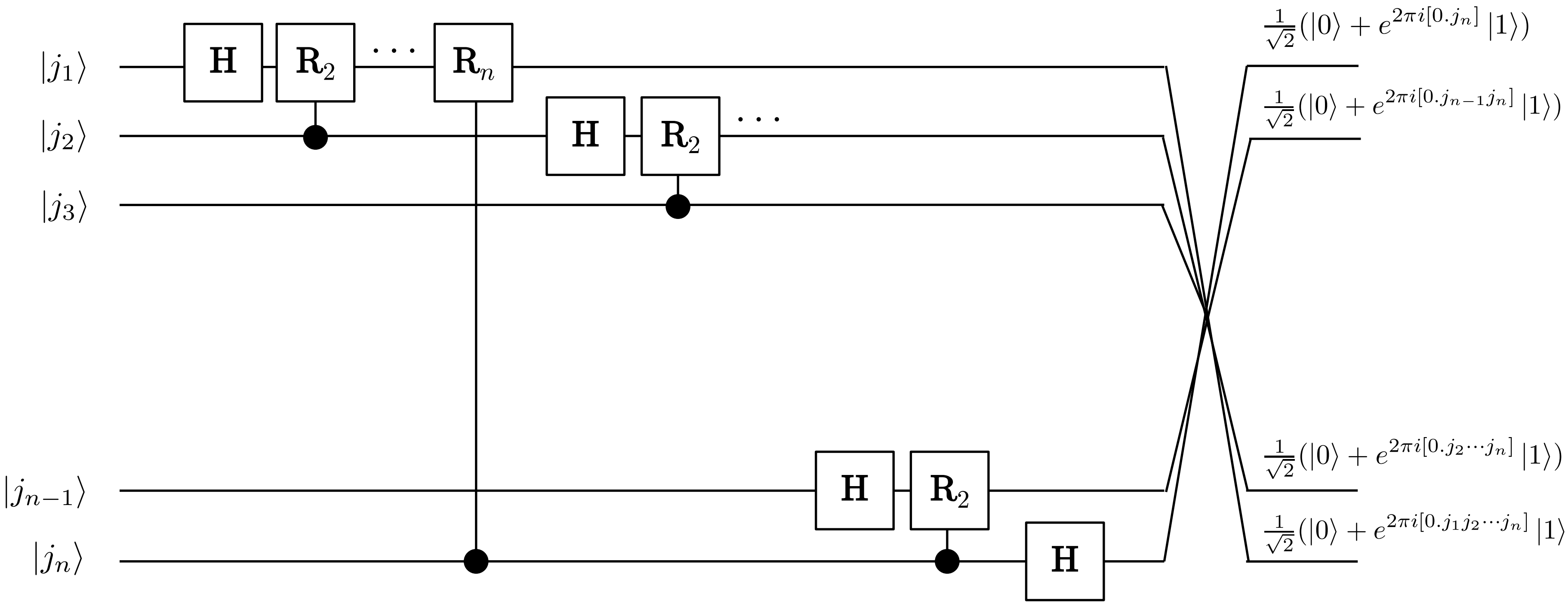
We therefore conclude that

$$\mathrm{QFT}(|j_1 j_2 \cdots j_n\rangle) =$$

$$\frac{1}{\sqrt{N}}\left(|0\rangle + e^{2\pi i[0.j_n]}|1\rangle\right) \otimes \left(|0\rangle + e^{2\pi i[0.j_{n-1}j_n]}|1\rangle\right) \otimes \cdots \otimes \left(|0\rangle + e^{2\pi i[0.j_1 j_2 \cdots j_n]}|1\rangle\right)$$

$$\mathbf{H}|0\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle\,,\ \mathbf{H}|1\rangle = \frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle$$

$$\mathbf{R}_l = \begin{bmatrix} 1 & 0 \\ 0 & e^{\frac{2\pi i}{2^l}} \end{bmatrix}$$



Quantum Fourier transform $\sim O(n^2)$ gates

Classical Fourier transform $\sim O(n2^n)$ gates

Annealing quantum processors [edit]

These QPUs are based on quantum annealing.

Manufacturer	Name/Codename/Designation	Architecture	Layout	Socket	Fidelity	Qubits	Release date
D-Wave	D-Wave One (Ranier)	Superconducting	N/A	N/A	N/A	128 qb	11 May 2011
D-Wave	D-Wave Two	Superconducting	N/A	N/A	N/A	512 qb	2013
D-Wave	D-Wave 2X	Superconducting	N/A	N/A	N/A	1152 qb	2015
D-Wave	D-Wave 2000Q	Superconducting	N/A	N/A	N/A	2048 qb	2017
D-Wave	D-Wave Advantage	Superconducting	N/A	N/A	N/A	5000 qb	2020

Wikipedia

Circuit-based quantum processors [edit]

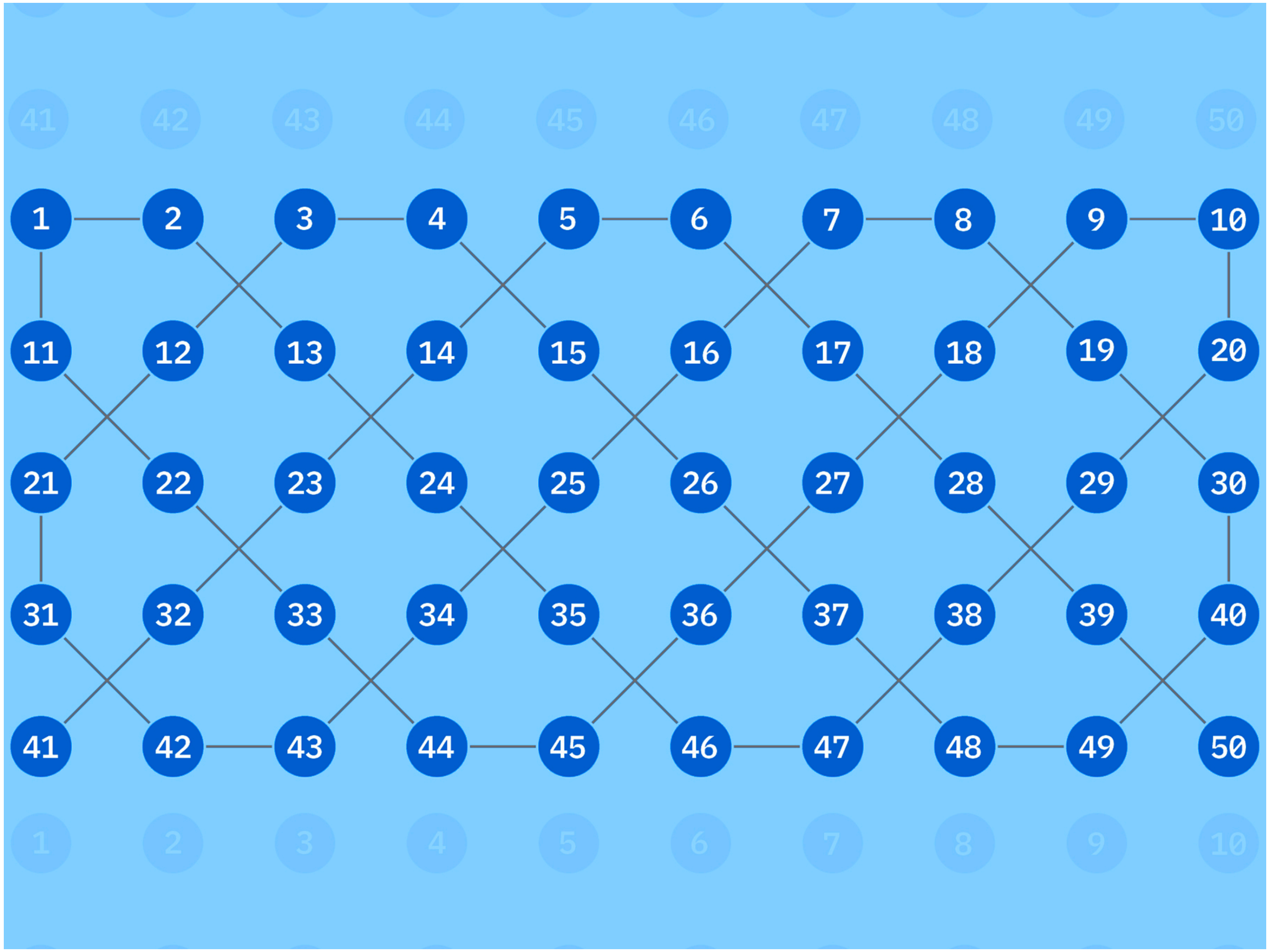
These QPUs are based on the quantum circuit and quantum logic gate-based model of computing.

Manufacturer	Name/Codename/Designation	Architecture	Layout	Socket	Fidelity	Qubits	Release date
Google	N/A	Superconducting	N/A	N/A	99.5%[1]	20 qb	2017
Google	N/A	Superconducting	7×7 lattice	N/A	99.7%[1]	49 qb[2]	Q4 2017 (planned)
Google	Bristlecone	Superconducting	6×12 lattice	N/A	99% (readout) 99.9% (1 qubit) 99.4% (2 qubits)	72 qb[3][4]	5 March 2018
Google	Sycamore	Nonlinear superconducting resonator	N/A	N/A	N/A	54 transmon qb 53 qb effective	2019
IBM	IBM Q 5 Tenerife	Superconducting	bow tie	N/A	99.897% (average gate) 98.64% (readout)	5 qb	2016[1]
IBM	IBM Q 5 Yorktown	Superconducting	bow tie	N/A	99.545% (average gate) 94.2% (readout)	5 qb	
IBM	IBM Q 14 Melbourne	Superconducting	N/A	N/A	99.735% (average gate) 97.13% (readout)	14 qb	
IBM	IBM Q 16 Rüschlikon	Superconducting	2x8 lattice	N/A	99.779% (average gate) 94.24% (readout)	16 qb[5]	17 May 2017 (Retired: 26 September 2018)[6]
IBM	IBM Q 17	Superconducting	N/A	N/A	N/A	17 qb[5]	17 May 2017
IBM	IBM Q 20 Tokyo	Superconducting	5x4 lattice	N/A	99.812% (average gate) 93.21% (readout)	20 qb[7]	10 November 2017
IBM	IBM Q 20 Austin	Superconducting	5x4 lattice	N/A	N/A	20 qb	(Retired: 4 July 2018)[6]
IBM	IBM Q 50 prototype	Superconducting	N/A	N/A	N/A	50 qb[7]	
IBM	IBM Q 53	Superconducting	N/A	N/A	N/A	53 qb	October 2019
Intel	17-Qubit Superconducting Test Chip	Superconducting	N/A	40-pin cross gap	N/A	17 qb[8][9]	10 October 2017
Intel	Tangle Lake	Superconducting	N/A	108-pin cross gap	N/A	49 qb [10]	9 January 2018
Rigetti	8Q Agave	Superconducting	N/A	N/A	N/A	8 qb	4 June 2018[11]
Rigetti	16Q Aspen-1	Superconducting	N/A	N/A	N/A	16 qb	30 November 2018[11]
Rigetti	19Q Acorn	Superconducting	N/A	N/A	N/A	19 qb[12]	17 December 2017
IBM	IBM Armonk[13]	Superconducting	Single Qubit	N/A	N/A	1 qb	16 October 2019
IBM	IBM Ourense[13]	Superconducting	T	N/A	N/A	5 qb	03 July 2019
IBM	IBM Vigo[13]	Superconducting	T	N/A	N/A	5 qb	03 July 2019
IBM	IBM London[13]	Superconducting	T	N/A	N/A	5 qb	13 September 2019
IBM	IBM Burlington[13]	Superconducting	T	N/A	N/A	5 qb	13 September 2019
IBM	IBM Essex[13]	Superconducting	T	N/A	N/A	5 qb	13 September 2019

Wikipedia

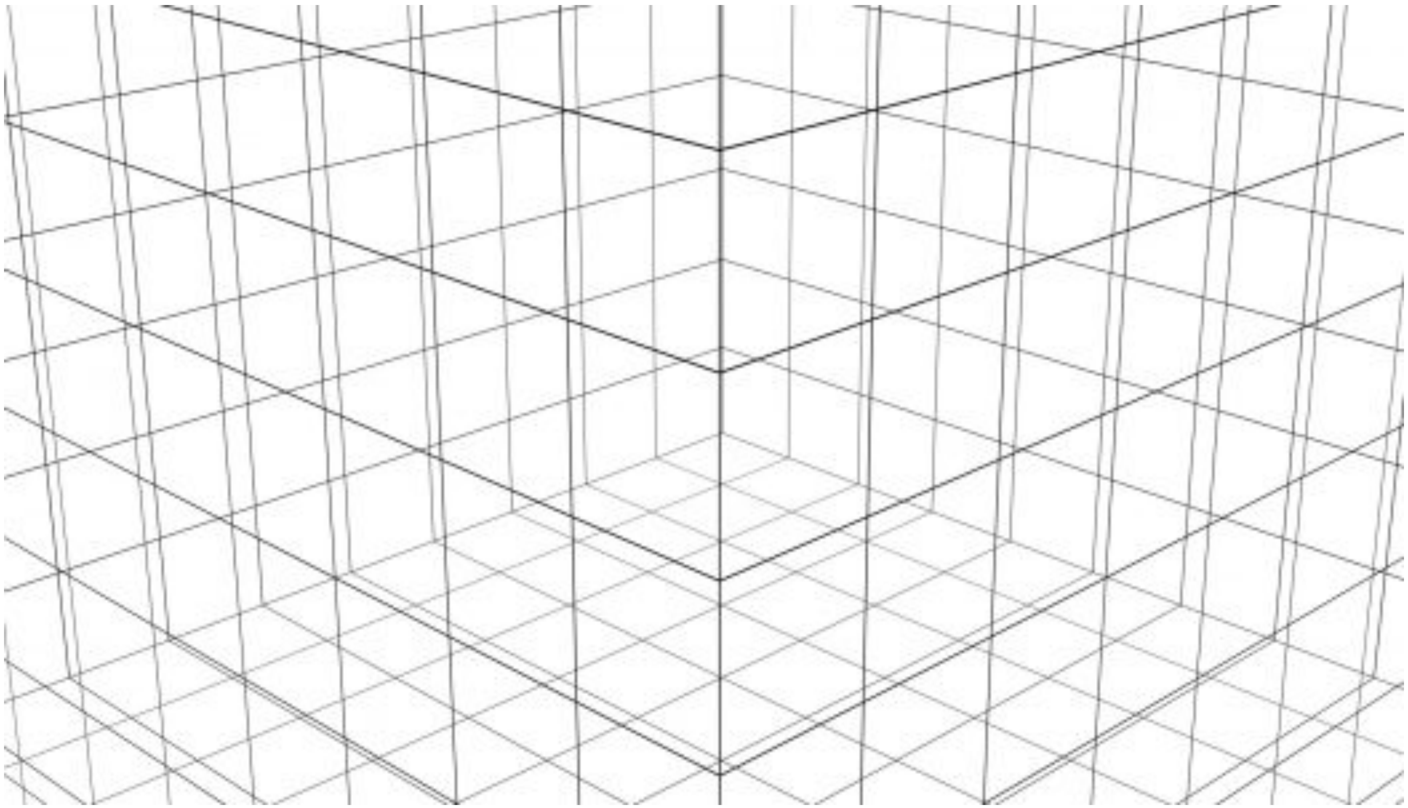
	Tenerife	Tokyo	Poughkeepsie	System One
Two-qubit CNOT error rate	4.02%	2.84%	2.25%	1.69%
Single qubit error rate	0.17%	0.20%	0.11%	0.04%

IBM Q


41
42
43
44
45
46
47
48
49
50
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
1
2
3
4
5
6
7
8
9
10

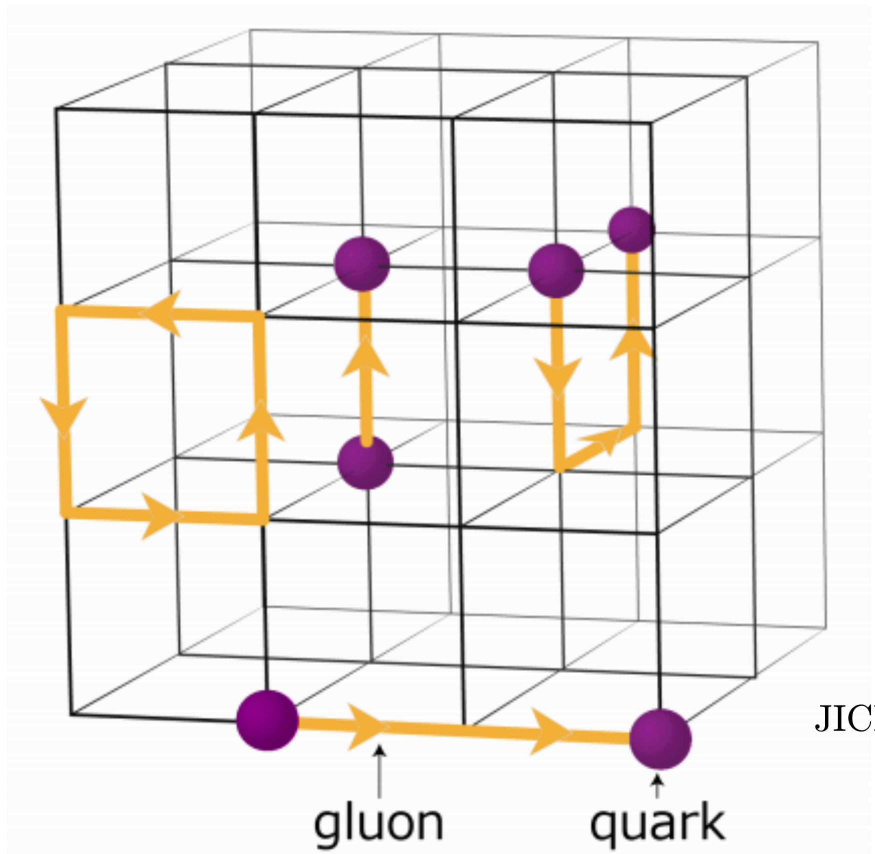
IBM Q

Lattice methods for nuclear physics



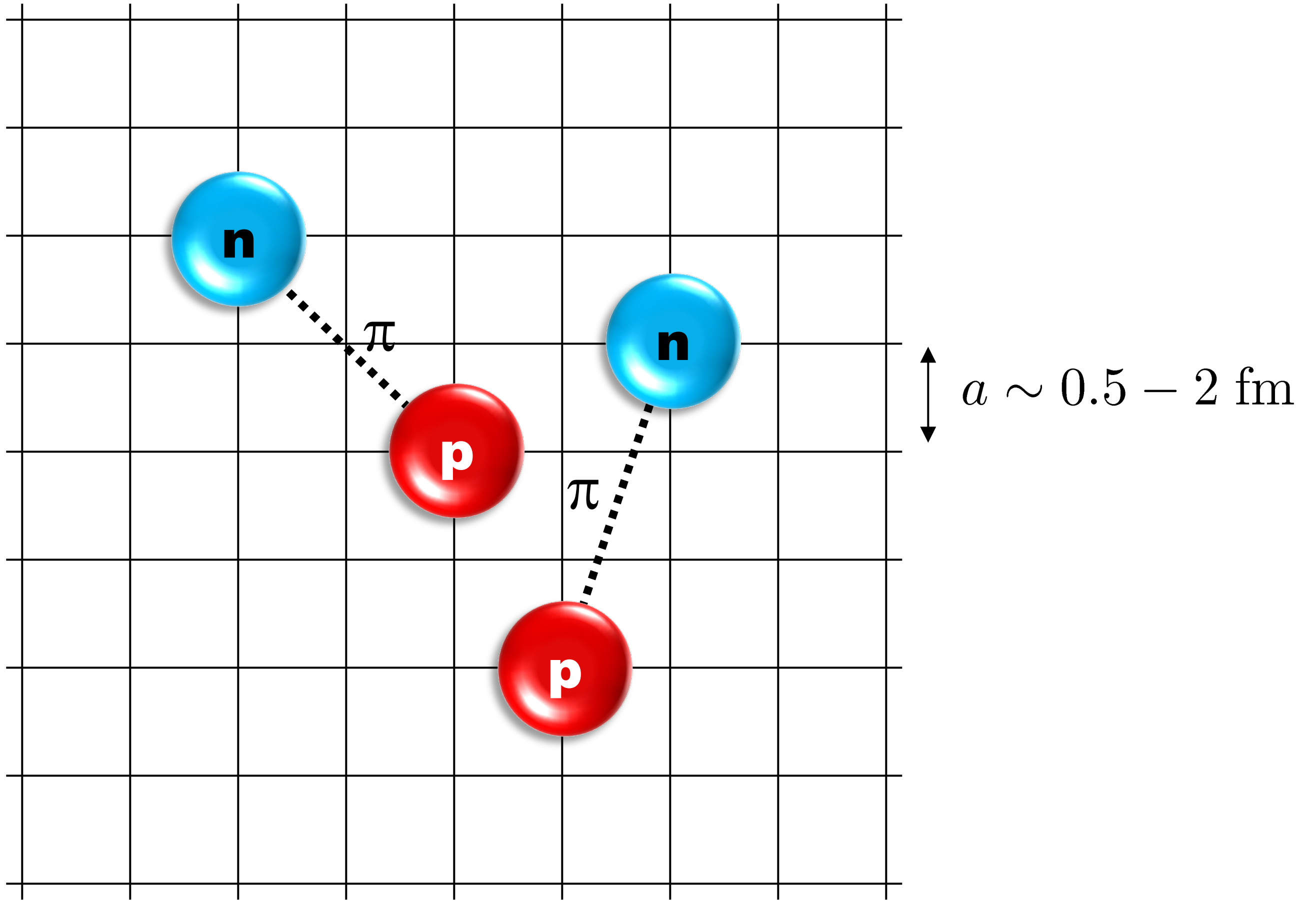
ORNL

<u>Lattice quantum chromodynamics</u>



JICFuS, Tsukuba

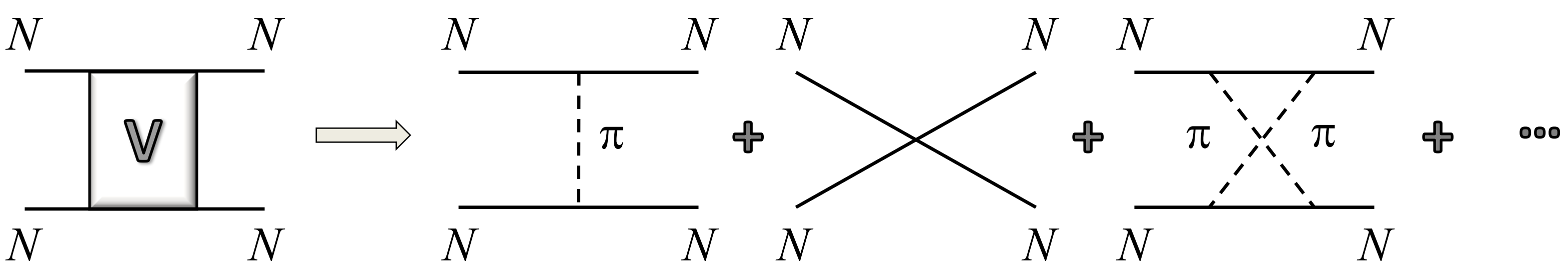
Lattice effective field theory



Review: D.L, Prog. Part. Nucl. Phys. 63 117-154 (2009)
Springer Lecture Notes: Lähde, Meißner, "Nuclear Lattice Effective Field Theory" (2019)

Chiral effective field theory

Construct the effective potential order by order

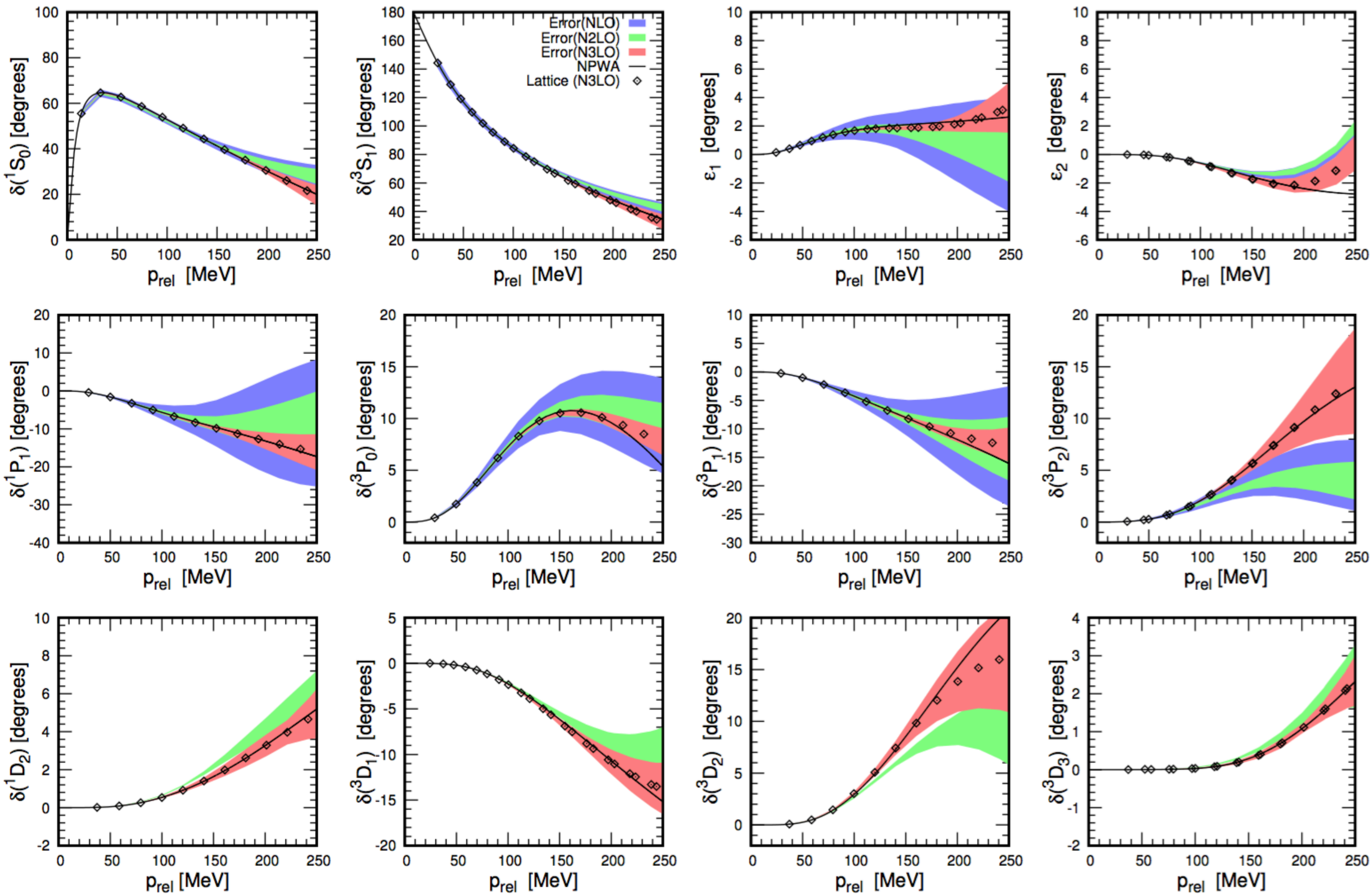


V^{OPEP} Contact interactions V^{TPEP}

Leading order (LO) Next-to-leading order (NLO)

$a = 1.315\,\mathrm{fm}$

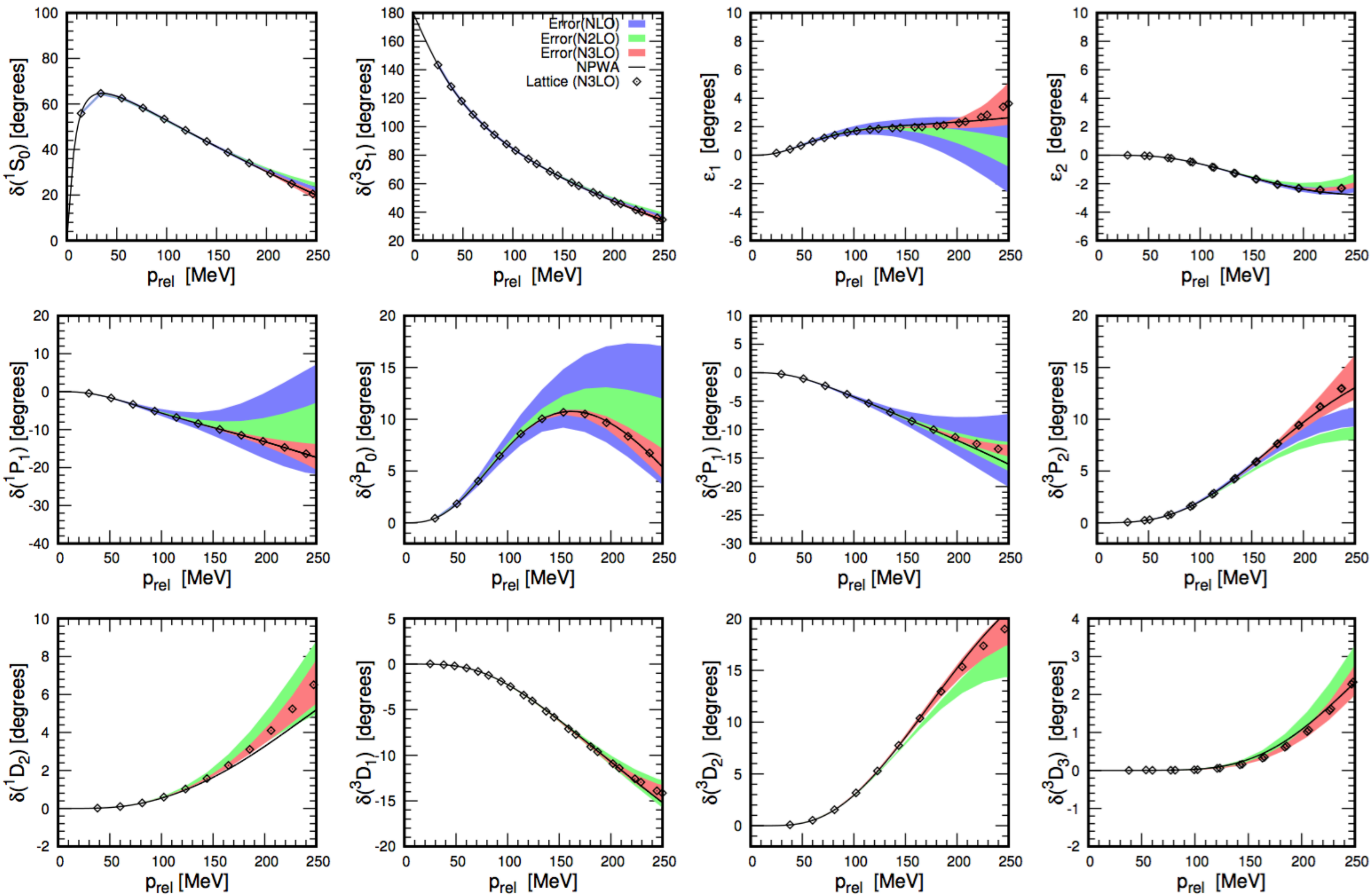
Figures by Ning Li



Li, Elhatisari, Epelbaum, D.L., Lu, Meißner, PRC 98, 044002 (2018)

$a = 0.987\,\mathrm{fm}$

Figures by Ning Li



Li, Elhatisari, Epelbaum, D.L., Lu, Meißner, PRC 98, 044002 (2018)

Recap of lecture

Qubits

Bloch sphere

Single-qubit gates

Two-qubit gates

Jordan-Wigner transformation

Quantum Fourier transform

Quantum circuits and performance

Lattice methods for nuclear physics